

**Final Report for Period:** 06/2010 - 05/2011**Submitted on:** 10/20/2011**Principal Investigator:** Yeung, Pui-Kuen .**Award ID:** 0553867**Organization:** Georgia Tech Research Corp**Submitted By:**

Yeung, Pui-Kuen - Principal Investigator

**Title:**

Collaborative Research: Large Numerical Simulations of Turbulence and Reynolds, Schmidt and Rossby Number Scalings

**Project Participants****Senior Personnel****Name:** Yeung, Pui-Kuen**Worked for more than 160 Hours:** Yes**Contribution to Project:****Name:** Sreenivasan, Katepalli**Worked for more than 160 Hours:** No**Contribution to Project:**

Professor Sreenivasan is the PI of the collaborating proposal (CBET-0553602) which is funded jointly with the PI's present grant. He has worked with us closely on many issues of physical interpretation and theoretical understanding based on the numerical simulation results.

**Name:** Sawford, Brian**Worked for more than 160 Hours:** No**Contribution to Project:**

Dr. Sawford is a leading authority in turbulent dispersion modeling, and currently an Adjunct Professor at Monash University, Australia. He has worked closely with the PI and his student (Jason Hackl) on the analysis and interpretation of numerical simulation data for two-particle Lagrangian statistics.

**Post-doc****Graduate Student****Name:** Donzis, Diego**Worked for more than 160 Hours:** Yes**Contribution to Project:**

Mr Donzis is partially supported by the present grant. He has played a very important role in many tasks, including code development, conduct of large simulations, and the analysis of numerical simulation data. He has interacted closely with IBM staff at IBM Watson Research Center in testing a new simulation code using up to 32768 processors on the Currently World's No. 3 IBM Blue Gene at Watson.

**Name:** Hackl, Jason**Worked for more than 160 Hours:** Yes**Contribution to Project:**

Mr Jason Hackl is partially supported by the present NSF grant. He has worked on two-particle Lagrangian statistics, including new analyses of "exit-time" results, using the resources of San Diego and Pittsburgh Supercomputer Centers.

**Name:** Iyer, Kartik

**Worked for more than 160 Hours:** Yes

**Contribution to Project:**

Mr Iyer is a graduate student supported by internal institutional funds. He is relatively new in the project and has been mainly spending time learning to use the various software tools available. He is also working with researchers from France who would like to use our simulation data for purposes of wavelet analyses and Coherent Vortex Simulation.

**Undergraduate Student**

**Technician, Programmer**

**Other Participant**

**Research Experience for Undergraduates**

**Organizational Partners**

**San Diego Supercomputer Center**

San Diego Supercomputer Center (SDSC) has provided a total of 2.8 million processor hours as well as 40 Terabytes of Data Collections space on their machines during the current project year. Strategic consultants at SDSC have made vital contributions in a restructured simulation code which is capable of scaling up to very large numbers of processors, and necessary for future production simulations at grid resolutions  $4096^3$  and higher. SDSC staff also provided background support for benchmarking studies on a larger machine at IBM Watson Research Center.

**Pittsburgh Supercomputing Center**

Pittsburgh Supercomputing Center (PSC) has provided roughly 1 million processor hours on their machines for the current budget year. A strategic consultant has provided valuable assistance for porting codes to new machines.

**IBM Watson Research Center**

IBM Watson Research Center has provided time for testing and benchmarking for our new simulation code on their 40960-processor Blue Gene/L supercomputer (BGW for short) which is currently No. 3 on the list of the world's fastest supercomputers. The PI's PhD student visited IBM Watson in July 2006 as part of a selective 'Consortium Days' program. The PI himself also visited in April 2007 and held discussions with several members of the Blue Gene applications development team.

**Texas Advanced Computing Center**

Some of the largest computations were performed using the machine 'Ranger' operated by Texas Advanced Computing Center (TACC, at University of Texas at Austin) which received the first NSF "Track 2" Award. TACC staff also provided assistance in operations and performance optimization.

### **National Institute for Computational Sci**

Some of the largest computations in 2008-2009 were performed on the 'Kraken' machine at the National Institute for Computational Sciences (NICS), which is operated by the University of Tennessee at Oak Ridge National Laboratories and received the second NSF ``Track 2'' award. NICS staff also provided assistance in operations and performance optimization.

### **National Center for Computational Scienc**

The NCCS (operated by DoE Oak Ridge National Labs) provided 10 million hours of CPU time on their Cray XT supercomputers through a Petascale Early Science Program in 2009. In addition they provided an INCITE award of 20 million hours in 2010.

### **Other Collaborators or Contacts**

Dr. Dmitry Pekurovsky, a strategic consultant at SDSC, has had a major role in our recent code development efforts aimed at enabling future simulations at 4096<sup>3</sup> simulations and beyond.

The following researchers have participated in analyzing the data or have begun preliminary steps in the process:

- 1/ Prof. Brian L Sawford, Monash University, Australia
- 2/ Prof. Prosenjit Bagchi, Rutgers University, NJ
- 3/ Prof. Kai Schneider, France

Several others have made inquiries on the availability and appropriateness of our simulation data for their research interests.

### **Activities and Findings**

**Research and Education Activities:** (See PDF version submitted by PI at the end of the report)

**Findings:** (See PDF version submitted by PI at the end of the report)

#### **Training and Development:**

Two PhD students have completed their thesis work at Georgia Tech as a result of the funded research.

The first of these (Diego Donzis) graduated in 2007. After two years as postdoctoral fellow with K.R. Sreenivasan he has become an assistant professor at Texas A&M University in Fall 2009. He is an author or co-author of 7 journal manuscripts listed in this report.

The second (Jason Hackl, an US citizen) benefitted also from an IREE international training supplement and graduated in 2011. He is an author of two journal publications (including one where he was the primary author).

A third PhD student (Kartik Iyer) also received partial support from this grant. To date he has been co-author on one journal publication and has presented his work at a national conference in our field of research.

#### **Outreach Activities:**

#### **Journal Publications**

D.A. Donzis, P.K Yeung and K.R. Sreenivasan, "Energy dissipation rate and enstrophy in isotropic turbulence: resolution effects and scaling in direct numerical simulationsscaling and resolution effects in direct numerical simulations", *Physics of Fluids*, p. 045108, vol. 20, (2008). Published,

B.L. Sawford, P.K Yeung and J.F. Hackl, "Reynolds number dependence of relative dispersion statistics in isotropic turbulence", *Physics of Fluids*, p. 065111, vol. 20, (2008). Published,

D.A. Donzis, P.K. Yeung, "Resolution effects and scaling in numerical simulations of passive scalar mixing in turbulence", *Physica D*, p. 1278, vol. 239, (2010). Published,

D.A. Donzis, K.R. Sreenivasan, "Short-term forecasts and scaling of intense events in turbulence", *J. Fluid Mech.*, p. 199, vol. 647, (2010). Published,

B.L. Sawford and P.K Yeung, "Conditional relative acceleration statistics and relative dispersion modeling", *Flow, Turbulence and Combustion*, p. , vol. 85, (2010). Published, 10.1007/s10494-010-9271-6

D.A. Donzis, K.R. Sreenivasan and P.K Yeung, "The Batchelor spectrum for mixing of passive scalars in isotropic turbulence", *Flow, Turbulence and Combustion*, p. 549, vol. 86, (2010). Published, 10.1007/s10494-010-9254-7

D.A. Donzis, K.R. Sreenivasan, "The bottleneck effect and the Kolmogorov constant in isotropic turbulence", *J. Fluid Mech.*, p. , vol. 657, (2010). Published,

B. Kadoch, K.P. Iyer, D.A. Donzis, K. Schneider, M. Farge and P.K. Yeung, "On the role of vortical structures for turbulent mixing using direct numerical simulation and wavelet-based coherent vortex extraction.", *J. Turbulence*, p. , vol. 12, (2011). Published, doi:10.1080/14685248.2011.562511

Hackl, JF; Yeung, PK; Sawford, BL, "Multi-particle and tetrad statistics in numerical simulations of turbulent relative dispersion", *PHYSICS OF FLUIDS*, p. , vol. 23, (2011). Published, 10.1063/1.358680

Donzis, D.A; Sreenivasan, K.R.; Yeung, P.K., "Some results on the Reynolds number scaling of pressure statistics in isotropic turbulence.", *Physica D*, p. , vol. , (2011). Accepted, 10.1016/j.physd.2011.04.015

Blum, D.B., Bewley, G.P., Bodenschatz, E., Gilbert, M., Gylfason, A., Mydlarski, L., Voth, G.A., Xu, H. and Yeung, P.K., "Signatures of non-universal large scales in conditional structure functions from various turbulent flows", *New Journal of Physics*, p. , vol. , (2011). Accepted,

Sawford, B.L. and Yeung, P.K., "Kolmogorov similarity scaling for one-particle Lagrangian statistics.", *Physics of Fluids*, p. 091704, vol. 23, (2011). Published,

#### **Books or Other One-time Publications**

D.A. Donzis, "Scaling of Turbulence and Turbulence Mixing Using Terascale Numerical Simulations", (2007). Thesis, Published Bibliography: PhD Thesis, School of Aerospace Engineering, Georgia Institute of Technology

D.A. Donzis, P.K. Yeung,  
D. Pekurovsky, "Turbulence simulations on  $10^4$  processors", (2008). conference paper, Published  
Bibliography: Science Track paper, TeraGrid'08  
Conference, Las Vegas, NV, June 2008

P.K. Yeung, D.A. Donzis and K.R. Sreenivasan, "Pressure fluctuations and small-scale intermittency in DNS at high Reynolds number.", (2009). conference proceedings,  
Bibliography: Proceedings of Euromech Colloquium on "Small-scale turbulence and related gradient statistics" (Turin, Italy; October 2009)

P.K. Yeung, K.R. Sreenivasan and D.A. Donzis, "On the intermittency of dissipation rates in high-resolution simulations of turbulent mixing", (2010). conference proceedings, Published  
Bibliography: Session on Non-Classical  
Turbulence Physics,  
U.S National Congress of Theoretical and Applied Mechanics,  
University Park, PA, June-July 2010.

P.K. Yeung, "Lagrangian statistics of velocity gradients at high Reynolds number", (2010). conference proceedings, Published  
Bibliography: Session on High Reynolds  
Number Turbulence,  
U.S National Congress of Theoretical and Applied Mechanics,  
University Park, PA, June-July 2010.

Hackl, J.F., "Fixed-scale statistics and the geometry of turbulent dispersion at high Reynolds number via numerical simulation.", (2011).  
Thesis, Published  
Bibliography: PhD Thesis, School of Aerospace Engineering, Georgia Institute of Technology

Gotoh, T; Yeung, P.K, "Passive scalar transport in turbulence: a computational perspective.", (2011). Book, Accepted  
Editor(s): Davidson, P.A.; Kaneda, Y.;  
Sreenivasan, K.R.  
Collection: The Nature of Turbulence  
Bibliography: Chap 7  
Cambridge University Press

### Web/Internet Site

### Other Specific Products

### Contributions

#### **Contributions within Discipline:**

We are making a sustained effort to work with a number of researchers who have indicated interest in our large database from past and recent simulations at various problem sizes.

#### **Contributions to Other Disciplines:**

We have been active in the high-performance computing and Cyberinfrastructure community. The demanding requirements of our codes have helped motivate the improvement of software strategies at leading supercomputer sites. In developing the pencils version of our simulation code consultants at SDSC

have also generated a new module for three-dimensional Fourier transforms adaptable to machines with large number of processors. This FFT module has been tested by many researchers working in different fields of science, including many from abroad.

#### **Contributions to Human Resource Development:**

Together with institutional funds, this project has provided support and opportunities for three graduate students, including one US citizen and two international students. The first student completed his PhD thesis in August 2007 and is now (since Aug 2009) a faculty member at Texas A&M University. The second student, who is an American citizen, successfully defended his thesis in May 2011. The third is expected to present his thesis proposal by January 2012. The second student also benefitted from supplemental IREE funds which supported a three-month stay at Monash University, Australia in the summer of 2008.

#### **Contributions to Resources for Research and Education:**

A SDSC visualization specialist working with us has generated a 10-second dynamic animation of three-dimensional contour surfaces from a large simulation dataset. The video was submitted to the Multi-Media Fluid Mechanics project which is focused on educational purposes especially at the undergraduate level.

#### **Contributions Beyond Science and Engineering:**

### **Conference Proceedings**

#### **Categories for which nothing is reported:**

Activities and Findings: Any Outreach Activities

Any Web/Internet Site

Any Product

Contributions: To Any Beyond Science and Engineering

Any Conference

## Research Activities

*Note: Grant CBET-0553867 (PI: P.K. Yeung) was awarded concurrently in a collaborative arrangement with Grant 0553602 (PI: K.R. Sreenivasan) in 2006. We have worked closely and our names have appeared jointly in a majority of publications from the funded research. In this report we summarize all work performed jointly and/or under each PI's supervision.*

Broadly speaking, the main objectives of our project were (1) to advance understanding of turbulence scaling by analyzing data from direct numerical simulations (DNS), and (2) to advance our grid resolution to  $4096^3$  and make data available to the research community with assistance from supercomputer centers supported by NSF. Since the grant began in June 2006 we have made progress on several fronts, including successful conduct of three  $4096^3$  computations at three major supercomputing sites supported by NSF and DOE.<sup>1</sup> PK Yeung also leads two other projects supported by NSF's Office of Cyberinfrastructure, under the "PetaApps" (nsf07559) and PRAC (nsf08529) solicitations. The first of these two is a regular grant focused on development of Petascale algorithms; the second provides access to the NSF "Track 1" Petascale machine and support for related travel. This machine, now known as Blue Waters, will provide the computing power needed for future simulations at  $8192^3$  resolution. It is scheduled to be in production by the Summer of 2012, at the University of Illinois, Urbana-Champaign.

With approval from NSF, our project has seen two one-year no-cost extensions. The main reason for these extensions is that time is needed to analyze the very large datasets generated from our simulations. The pace of our progress is also subject to the need to apply competitively for many millions of CPU processor hours on an annual basis. Nevertheless we have made significant scientific contributions, which have formed the substance of 12 journal publications in print or in press, one review-type book chapter, as well as numerous presentations at public and invitation-only conferences, and invited seminars in various settings. In addition, K.R. Sreenivasan has used our science results in a number of invited lectures, most recently for a review lecture at the Turbulence Colloquium Marseille 2011 (France), which was an international gathering of senior researchers and young scholars in commemoration of a historically significant conference 50 years ago at the same location. While most of our publication efforts were already listed in our previous annual reports, since the date of our last report (August 2010) four new journal articles (Hackl *et al.* 2011, Donzis *et al.* 2011, Sawford & Yeung 2011, Blum *et al.* 2011) have originated and have reached published or accepted status.

Our work is well recognized in the high performance computing community, and has been featured in publicity articles that appeared on the websites of several leading HPC centers. We received a "5K Club" award certificate based on a conference manuscript at the TeraGrid Conference in June 2008. Our work has been featured in the 2008 TeraGrid Science Highlights publication, [<http://www.teragrid.org/news/sci-high08/whirlwind.html>]. We have also been active in serving both the fluid dynamics and high-performance computing communities: e.g, P.K. Yeung was the lead organizer of a Cyber Fluid Dynamics workshop at NSF in July 2007, was a member of the TeraGrid Science Advisory Board (2008-2010), and is currently a member of an external advisory committee for a Technology Audit Services project which is funded under NSF's Extreme Digital (XD) programs.

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<sup>1</sup>These three sites are: 1. Texas Advanced Computing Center [TACC] at Austin, TX; 2. National Institute for Computational Sciences [NICS] at University of Tennessee, Oak Ridge, TN; 3. National Center for Computational Sciences [NICS] at Oak Ridge National Labs., Oak Ridge, TN.

We summarize below the progress that we have made on several major aspects of this project. It should be noted that although the project has formally ended we will continue to maintain and analyze many hundreds of Terabytes of data archived, and hence more publication and dissemination efforts are planned.

## Computational issues and resources

We have enjoyed much success in algorithmic development and competitive resource allocations processes at the scale which makes  $4096^3$  simulations feasible. As reported in previous project years a key strategy is a domain decomposition scheme (Donzis, Yeung & Pekurovsky 2008) that divides an  $N^3$  grid along two coordinate directions instead of one, with the basic unit of data worked on by each processor being a “pencil” instead of a “slab”. This code allows the use of up to  $N^2$  processors and has served us well in the current generation of leading-edge supercomputers based on massively parallel processors. While the next-generation innovations are already on the horizon, our production codes are so-called pure MPI codes which distribute the memory among different processors and use the standard Message Passing Interface software library for interprocessor communications. A number of codes for post-processing, which is a vital step in the process of knowledge discovery, are also based on the same data structure and maintained using a modularized software library approach which will ultimately be helpful in sharing our codes with other interested parties in our research community.

PK Yeung has a long history of involvement with national supercomputer centers supported by NSF and/or DOE, and probably has received more allocations (over 80 million hours in the life of this project) than most other turbulence researchers in the US. In 2007 and 2008 we were selected to participate in “early-user” programs on both of the first two “Track 2” systems funded by NSF, in Texas and Tennessee. This has allowed us to build closer working relationships with the systems staff and to identify strategies for performance enhancement earlier than otherwise, while we made contributions to the user community by helping to identify systems issues on new machines.

We have performed three  $4096^3$  simulations of substantial length in time. The first simulation gives Lagrangian statistics of turbulent dispersion at Taylor-scale Reynolds number ( $R_\lambda$ ) about 1000. The second gives statistics of passive scalar mixing at  $R_\lambda \approx 650$  in a velocity field where the small scales are resolved better than most other authors in the literature have. The third is targeted at mixing of scalars with low molecular diffusivity, which is more demanding in resolution since smaller scales arise. To our knowledge, all of these simulations are the largest of their kind, worldwide.

In addition to production simulations at  $4096^3$ , we have benchmarked our codes at  $8192^3$  resolution on several machines, in particular using 131072 (128K) cores on a Cray XT5 (*Jaguarpf*) operated by NCCS at Oak Ridge, which based on its theoretical peak performance (2.3 Petaflops/s) is currently the third fastest supercomputer in the world (and fastest in the U.S). As one can expect, as the number of CPU cores used increases the time spent on interprocessor communication can increase significantly, which makes scalability harder to maintain, while risk of job failure due to hardware issues also grows.

As noted on p. 1, PK Yeung also leads two other projects funded by OCI at NSF. The first, under the PetaApps program, is a four-institution collaboration among three computation-oriented turbulence experts (R.D. Moser, U. Texas at Austin; J.J. Riley, U. of Washington) and three supercomputing specialists (D.A. Bader, Georgia Tech; A. Majumdar and D. Pekurovsky,



SDSC) to develop, and apply, state-of-the-art computing techniques to important canonical problems in turbulence. This includes additional physics (chemical reactions, buoyancy) and more complex yet canonical geometries (channels, boundary layers, free shear flows), all at Reynolds numbers as high as possible. The same team is also funded under the PRAC program to access the Blue Waters (the NSF Track 1 Petascale machine under development). NSF support on the science side is very important for maintaining our success in high-profile competitions where computing resources are in great demand.

## Reynolds number and intermittency

We have worked on a number of issues that provide important information about effects of Reynolds number and intermittency on various aspects of turbulence. A partial list includes resolution of the small scales, fluctuations of dissipation and enstrophy, Richardson scaling in Lagrangian relative dispersion, statistics of pressure fluctuations, the predictability of intense events, and “bottleneck” features in turbulence spectra. We have a number of publication efforts (published, in press, or under active preparation) to show, such as:

Donzis, Yeung & Sreenivasan (2008): We used simulations of nominally the same Reynolds number but different grid resolution to estimate, in some cases quantitatively, the effects of finite resolution (see Schumacher, Sreenivasan & Yeung 2005; Yakhot & Sreenivasan 2005) on various quantities of interest and hence to check whether previous conclusions in the literature based on DNS with moderate small-scale resolution are in need of revision. We also derived new estimates of the resolution needed to resolve structure functions of various orders, and reported on the occurrence of extreme and intermittent samples of dissipation and enstrophy at several thousand times of their mean values.

Sawford, Yeung & Hackl (2008): In this paper, also led by the PI’s collaborator Prof. B.L. Sawford (Monash University, Australia) we used DNS data at  $R_\lambda$  up to 1000 to examine the issue of Richardson inertial-range scaling for the dispersion of fluid particle pairs. Several different ways of assessing the value of Richardson’s constant were addressed. Our DNS database offers the advantages of more detailed information compared to experiment and higher Reynolds numbers than reported by other groups performing numerical simulations.

Donzis & Sreenivasan (2010a): We have studied the extent to which these large fluctuations can be predicted. In particular, we investigated the evolution of vorticity and the terms in its evolution equation. The results which, include a dynamical precursor for intense events, may be applicable to all intermittent quantities and have an even broader impact to other non-linear complex phenomena such as earthquakes.

Donzis & Sreenivasan (2010b): Using our extensive DNS database as well as new simulations at various resolutions and using different forcing schemes, we address the effect of these conditions over a wider range of Reynolds numbers than possible before. Of particular interest is the scaling of the bottleneck effect which is known to be problematic when the Kolmogorov constant needs to be determined from experimental and numerical data.

Sawford & Yeung (2010): In this paper, also led by Prof. B.L. Sawford, we used DNS data at  $R_\lambda$  up to 1000 (grid resolution  $4096^3$ ) to compute the statistics of longitudinal and transverse acceleration given, jointly, the corresponding velocity differences between two points in space. The objective is to explore the process by which effects of Eulerian

spatial intermittency can be incorporated into the modeling of dispersion between a pair of fluid particles in turbulent flow.

Hackl, Yeung & Sawford (2011): We used results from DNS to study the scaling behavior of multi-cluster evolution, and with a focus on comparing the scalings of measures of size versus measures of shape. Research leading to this paper started with a three-month visit in Australia, hosted by Prof. Sawford, of the PI's PhD student Jason Hackl under an NSF IREE supplement in summer 2008. This is also the core of student's thesis research, which concluded with a successful thesis defense in May 2011.

Donzis, Sreenivasan & Yeung (2011): We used DNS data at Taylor-scale Reynolds number up to 1000 to study the scaling of the amplitude and length scales of pressure fluctuations. We made observations concerning the ratio of both large and small scales of the pressure field compared to those of the velocity. Intermittency corrections are proposed to help explain the observed trends.

Sawford & Yeung (2011): We used results from DNS, in conjunction with a prediction from stochastic modeling, to address the issue of inference of Kolmogorov scaling for one-particle Lagrangian statistics. While unambiguous scaling in the second-order structure function has been difficult to obtain, it appears that the acceleration spectrum shows significantly better scaling. This result also suggests good prospects for studying Lagrangian similarity in a future  $8192^3$  DNS at Taylor-scale Reynolds number approximately 1600.

Blum *et al.* (2011): This is a collaborative paper written with several experimentalists interested in a comparison between numerical simulation and experiment. We used data from a  $2048^3$  simulation to compute conditional structure functions in an attempt to better understand the possible dependence of small-scales motion on large-scale flow features.

Yeung, Donzis & Sreenivasan (2011): We use the best-resolved DNS datasets available at Taylor-scale Reynolds number 140 to 1000 (on  $2048^3$  and  $4096^3$  grids) to perform a comparative study of the statistics of fluctuations of dissipation and enstrophy. We examine the joint statistics of these quantities, with special interest in whether extreme events in both tend to occur together. We also explore the implications of these results on the pressure field via the Laplacian of the pressure fluctuation.

## Schmidt number and the scalar dissipation

It is well accepted that (e.g. Yeung *et al.* 2002, 2005) passive scalar fields of Schmidt number unity have more high-wavenumber spectral content and are more intermittent than velocity fields at the same Reynolds number. Accordingly, resolution of the small scales (see paragraphs above) can be a concern, perhaps even more so than for the velocity field. In addition, it is important to recognize that other requirements arise if the Schmidt number is very large or very low compared to unity. In the case of high  $Sc$  (low diffusivity) the smallest scale in the scalar field, called Batchelor scale  $\eta_B = \eta Sc^{-1/2}$ , is smaller than the Kolmogorov scale and thus requires finer resolution than the velocity field. The most interesting scaling range is then the so-called viscous-convective range of scale sizes between  $\eta$  and  $\eta_B$ , which can be well achieved only if  $Sc \gg 1$ . In the case of low  $Sc$  (high diffusivity) the largest scales in the scalar field become larger than those of the velocity, thus calling for a larger domain size

(hence more grid points) in the simulations. Since high diffusivity implies very fast molecular diffusion a smaller time step size (hence more time steps) is also essential at the smaller scales.

To examine the effects of resolution for passive scalar statistics in DNS we have performed a number of simulations giving results at nominally the same Reynolds number and same Schmidt number but different grid resolutions. In Donzis & Yeung (2010) we assessed the effects of finite resolution in turbulent mixing in terms of the ratio of grid spacing to the Batchelor length scale for scalars of high Schmidt number. Special attention is paid to important trends concerning departure from local isotropy, and intermittency as a function of the Schmidt number. We have reported both the statistics of scalar gradient fluctuations and the effects of underresolution on observed intermittency exponents of scalar dissipation rate fluctuations. Incidentally, motivated by some issues in the analysis of relative dispersion we have also implemented a variant of the forcing scheme (Eswaran & Pope 1988) used to maintain the Reynolds number in previous work on isotropic turbulence. In Donzis & Yeung (2010) we also compared results from different forcing schemes.

Results in our earlier papers (Yeung, Xu, Donzis & Sreenivasan 2004) supported a classical theory by Batchelor (1959) which predicted that the spectrum of scalar fluctuations in the viscous-convective range (wavenumbers  $1/\eta \ll k \ll 1/\eta_B$ ) would have a  $k^{-1}$  functional form. However the earlier results were obtained at relatively low Reynolds numbers without inertial-range properties in the velocity field. To address this issue more rigorously we have performed a  $2048^3$  simulation with passive scalars at  $Sc = 4$  and  $64$  and velocity field at  $R_\lambda \sim 140$  which is at the value where inertial-range scaling begins to emerge in the Eulerian energy spectrum for the velocity field (Yeung & Zhou 1997). In Donzis, Sreenivasan & Yeung (2010) we have studied both the form of Batchelor’s spectrum and the scaling constant, known as Batchelor constant. In particular the connection between Batchelor scaling and the statistics of principal strain rates has been explored in some detail. We also compared our DNS data with a theory by Kraichnan (1968) which predicted a stretched exponential falloff in the viscous-diffusive range ( $k \gg 1/\eta_B$ ).

Our experience in studies of high Schmidt number mixing has suggested that asymptotic trends start to develop when  $Sc$  exceeds a certain value which is Reynolds number dependent. To test this hypothesis more completely we need some new data points in the  $Re-Sc$  parameter space. Accordingly to reach higher  $Sc$  at a higher Reynolds number we have performed a new simulation at  $4096^3$  resolution with  $R_\lambda \approx 240$  and  $Sc = 32$ . Because of an issue with numerical stability specific to high  $Sc$  we have performed this simulation using a fourth-order Runge-Kutta scheme for integration in time. Data from this simulation are in the process of being analyzed. Preliminary results have been obtained also for the case of very low Schmidt number and are being extended to higher Reynolds number.

PK Yeung has recently completed an invited book chapter (Gotoh & Yeung 2011) on studies of turbulent mixing with an emphasis on computations. This article is co-authored with a leading Japanese scientist and is to appear in an edited volume to be called *The Nature of Turbulence* which will be published by Cambridge University Press in the next few months. This article is written in the form of a review which summarizes recent research in the field and suggests new directions for future research. A central question is approach to asymptotic scaling which is examined separately for both low-order and high-order statistics.

In addition to the above core items on our research agenda we have also worked with a group in France (led by Profs. M. Farge and K. Schneider) known for use of wavelet methods and a technique called Coherent Vortex Simulation (CVS) which decomposes velocity fluctuations into a coherent part and an incoherent part. We have a joint paper published early this year (Kadoch *et al.* 2011) in which the effects of coherent and inherent motions on turbulent mixing

are examined separately.

## Rossby number and small-scale anisotropy

Because of other priorities and limitations in CPU allocations received, we have worked less in this areas than the others.

In previous work we presented numerical evidence that rotation leads to a strong degree of anisotropy and a reduction of intermittency in both the velocity field (Yeung, Xu & Sreenivasan 2003) and scalar field (Yeung & Xu 2004). However our results showed substantial statistical variability as well as symptoms of sensitivity to finite domain size. Accordingly in the (completed) PhD thesis work of Diego Donzis at Georgia Tech we have performed simulations with domain size  $(4\pi)^3$  instead of the usual  $(2\pi)^3$ . For characterizing the nature of intermittency in rotating turbulence we have also implemented new routines that successfully separate the so-called “directional” and “polarization” components of anisotropy at different scale sizes in the energy spectrum. A hypothesis of a “local” Taylor-Proudman theorem has been investigated.

## Data access and serving the research community

Making data *readily* accessible to the research community is an important goal for us. Previously we were allocated 40 Terabytes of “Data Collections” disk space for this purpose, at the San Diego Supercomputer Center. Access to the data was managed by the Storage Resource Broker utility (SRB, see <http://www.sdsc.edu/srb>) We also installed some SRB-related software onto our local Linux machines at Georgia Tech, and have learned how to organize our files and directories as well as to assign tickets (tokens) which other members of the research community can use to access the data. Several researchers approached us for access to our DNS database, and at least one paper has been published based on such analyses, with our indirect contributions prominently acknowledged in the manuscript. Papers led by other groups cited earlier in this report also provide evidence of the value of our data to the turbulent community, both in the US and abroad.

Admittedly, we would like to see our database being used by a yet larger number of research groups. We see a need for better publicity, and for improved user-friendliness in the handling of our very large datasets. The subject of data-intensive computing, and the long-term storage of large datasets, is one which is encroaching more and more on the HPC horizon. As of October 2011 we have been approved to receive assistance from consultants at NSF-supported supercomputer centers on how to consolidate and improve accessibility to our datasets using the latest (called iRODS) software which is replacing SRB).

During the term of our project PK Yeung has been very active in Cyber-oriented service to the turbulence community. He was the lead organizer of the “NSF Workshop on Cyber-Fluid Dynamics: New Frontiers in Research and Education”, held at NSF in July 2007, for which a final report containing many details and recommendations are available through an URL link from <http://www.nsf.gov/eng/cbet/workshops/>. Over the years this event has led to several other developments, including the formation of an ad-hoc committee on Cyber Fluid Dynamics in the American Physical Society, Division of Fluid Dynamics; and a Workshop on “Development of Fluid Mechanics Community Software and Data Resources”, also supported by NSF and held in March 2010. The work of the “CyberFD” ad-hoc committee has been

partly documented in the final project report of Grant CBET-0735157.

Further evidence of our group’s visibility in the NSF-sponsored HPC community is that D.A. Donzis, although still a young scholar (assistant professor at Texas A&M University since August 2009) has been serving as a member of Petascale User Committees for both TACC and NICS.

### Human resource development

Collaboration between the two PIs of this project (P.K Yeung and his collaborating PI, Prof. K.R. Sreenivasan) has been very fruitful regarding high-quality human resource development. In particular, P.K Yeung’s former PhD student D.A. Donzis, who completed his PhD thesis in 2007 and subsequently worked as postdoctoral fellow for 2 years with Prof. Sreenivasan, is now (since Fall 2009) a faculty member at a major research institution (Texas A&M University). Dr. Donzis has also received a highly competitive NSF Faculty Early Career Award, funded jointly by the Office of Cyberinfrastructure and the Fluid Dynamics Program. Two other PhD students have been trained in our research program. One (Jason Hackl, an US citizen) graduated in Summer 2011 and is (subject to a work visa application) expected to join a leading research group in Barcelona, Spain on intensive simulations of wall-bounded flows. The second (Kartik Iyer) has been gaining in exposure and experience in large-scale computing, and is expected to present his PhD thesis proposal by early 2012.

### Current and future outlook

Currently our work is continuing under NSF support through a one-year grant (CBET-1139037), entitled “EAGER: Reaching higher in numerical simulations of turbulence” funded by the Fluid Dynamics Program. Proposals for longer-term support are being planned for the next submission time window.

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## Research Findings

*For simplicity, while focusing on the scientific outcomes of our project, in lieu of extended descriptions we show below the abstracts of all journal articles resulting wholly or in part from the funded research that are published or accepted as of October 2011.*

DONZIS, D.A., YEUNG, P.K. & SREENIVASAN, K.R. (2008) Energy dissipation rate and enstrophy in isotropic turbulence: scaling and resolution effects in direct numerical simulations. *Phys. Fluids* **20**, 045108.

Existing experimental and numerical data suggest that the turbulent energy dissipation and enstrophy (i.e., the square of vorticity) possess different scaling properties, while available theory suggests that there should be no differences at sufficiently high Reynolds numbers. We have performed a series of direct numerical simulations with up to  $2048^3$  grid points where advanced computational power is used to increase the Reynolds number (up to 650 on the Taylor scale) or to resolve the small scales better (down to  $1/8$  of a Kolmogorov scale). Our primary goal is to assess the differences and similarities between dissipation and enstrophy. Special attention is paid to the effects of small-scale resolution on the quality and reliability of the data, in view of recent theoretical work [V. Yakhot & K.R. Sreenivasan, *J. Stat. Phys.*, **121**, 823 (2005)] which stipulates the resolution needed to obtain a moment of a given order. We also provide error estimates as a function of small-scale resolution. Probability density functions of dissipation and enstrophy at high Reynolds number reveal the presence of extreme events several thousands times of the mean. The extreme events in dissipation and enstrophy fields appear to scale alike, overlap substantially in space, and are nearly statistically isotropic, while fluctuations of moderate amplitudes, at least for the present Reynolds numbers, show persistent differences. Conditional sampling shows that intense dissipation is likely to be accompanied by similarly intense enstrophy, but intense enstrophy is not always accompanied by intense dissipation.

SAWFORD, B.L., YEUNG, P.K. & HACKL, J.F. (2008) Reynolds number dependence of relative dispersion statistics in isotropic turbulence. *Phys. Fluids* **20**, 065111 (12 pages).

Direct numerical simulation results for a range of relative dispersion statistics over Taylor-scale Reynolds numbers up to 650 are presented in an attempt to observe and quantify inertial subrange scaling and, in particular, Richardson's  $t^3$  law. The analysis includes the mean-square separation and a range of important but less-studied differential statistics for which the motion is defined relative to that at time  $t = 0$ . It seeks to unambiguously identify and quantify the Richardson scaling by demonstrating convergence with both the Reynolds number and initial separation. According to these criteria, the standard compensated plots for these statistics in inertial subrange scaling show clear evidence of a Richardson range but with an imprecise estimate for the Richardson constant. A modified version of the cube-root plots introduced by Ott and Mann [*J. Fluid Mech.* **422**, 207 (2000)] confirms such convergence. It has been used to yield more precise estimates for Richardson's constant  $g$  which decrease with Taylor-scale Reynolds numbers over the range of 140650. Extrapolation to the large Reynolds number limit gives an asymptotic value for Richardson's constant in the range  $g = 0.55 - 0.57$ , depending on the functional form used to make the extrapolation.

DONZIS, D.A. & SREENIVASAN, K.R. (2010a) Short-term forecasts and scaling of intense events in turbulence. *J. Fluid Mech.* **647**, 13-26.

Extreme events such as intense tornadoes and huge floods, though infrequent, are particularly important because of their disproportionate impact. Our ability to forecast them is poor at present. Large events occur also in intermittent features of turbulent flows. Some dynamical understanding of these features is possible because the governing equations are known and can be solved with good accuracy on a computer. Here, we study large-amplitude events of turbulent vorticity using results from direct numerical simulations of isotropic turbulence in conjunction with the vorticity evolution equation. We show that the advection is the dominant process by which an observer fixed to the laboratory frame perceives vorticity evolution on a short timescale, and that the growth of squared-vorticity during large excursions is quadratic in time when normalized appropriately. This result is not inconsistent with the multifractal description and is simpler for present purposes. Computational data show that the peak in the viscous term of the vorticity equation can act as a precursor for the upcoming peak of vorticity, forming a reasonable basis for forecasts on short timescales that can be estimated simply. This idea can be applied to other intermittent quantities and, possibly, more broadly to forecasting other extreme quantities, e.g., in seismology.

DONZIS, D.A. & SREENIVASAN, K.R. (2010b) The bottleneck effect and the Kolmogorov constant in isotropic turbulence. *J. Fluid Mech.* **657**, 171-188.

A large database from direct numerical simulations (DNS) of isotropic turbulence, including recent simulations for box-sizes of up to  $4096^3$  and Taylor Reynolds number  $R_\lambda \approx 1000$ , is used to investigate the bottleneck effect in three-dimensional energy spectrum and in second-order structure functions, and to determine the Kolmogorov constant,  $C_K$ . The difficulties in estimating  $C_K$  at any finite Reynolds number, introduced by intermittency and bottleneck, are assessed. The data conclusively show that the bottleneck effect decreases with the Reynolds number. On this basis, an alternative to the usual procedure for determining  $C_K$  is suggested; this proposal does not depend on the particular choices of fitting ranges or power-law behavior in the inertial range. Within the resolution of the numerical data,  $C_K$  thus determined is a Reynolds-number-independent constant of  $\approx 1.58$  in three dimensional spectrum. A simple model including non-local transfer is proposed to reproduce the observed scaling features of the bottleneck.

DONZIS, D.A. & YEUNG, P.K. (2010) Resolution effects and scaling in numerical simulations of passive scalar mixing in turbulence. *Physica D* **239**, 1278-1287.

The effects of finite grid resolution on statistics of the small scales in direct numerical simulations of turbulent mixing of passive scalars are addressed in this paper. Simulations at up to  $2048^3$  grid points with grid spacing  $\Delta x$  varied from about 2 to  $1/2$  Batchelor scales ( $\eta_B$ ) show that most conclusions on Schmidt number ( $Sc$ ) dependence from prior work at less stringent resolution remain qualitatively correct, although simulations at resolution  $\Delta x \approx \eta_B$  are preferred and will give adequate results for many important quantities including the scalar dissipation intermittency exponent and structure functions at moderately high orders. For  $Sc \geq 1$ , since  $\eta_B = \eta Sc^{-1/2}$  (where  $\eta$  is the Kolmogorov scale), the requirement  $\Delta x \approx \eta_B$  is more stringent than the corresponding criterion  $\Delta x \approx \eta$  for the velocity field, which is thus well resolved in simulations aimed at high Schmidt number mixing. A simple argument is given to help interpret the effect of Schmidt and



Reynolds numbers on trends towards local isotropy and saturation of intermittency at high Schmidt number. The present results also provide evidence for a trend to isotropy at high Reynolds number with fixed  $Sc = 1.0$ . This is a new observation apparently not detected in less well resolved simulations in the past, and will require further investigation in the future.

SAWFORD, B.L. & YEUNG, P.K. (2010) Conditional relative acceleration statistics and relative dispersion modeling. *Flow, Turb. & Combust.* **85**, 349-362.

We have used DNS results for the Eulerian velocity difference probability density function and the mean acceleration difference conditioned on the velocity difference, to explore some of the assumptions underlying the formulation of Lagrangian stochastic models for relative dispersion. We focussed on the ability of the models to quantitatively represent Richardson's  $t^3$ -law and in particular the value of Richardson's constant. As a result of intermittency, with decreasing separation and with increasing Reynolds number these Eulerian quantities become more extreme and the model predictions for Richardson's constant also become more extreme (larger). This is in contrast with recent numerical simulations showing that Richardson's constant depends only weakly on Reynolds number. We conclude that, at least in the present Lagrangian stochastic modelling framework, in two-particle models (and presumably in multi-particle models) intermittency must be included explicitly in the dissipation rate as well as in the relative velocity statistics.

DONZIS, D.A., SREENIVASAN, K.R. & YEUNG, P.K. (2010) The Batchelor spectrum for mixing of passive scalars in isotropic turbulence. *Flow, Turb. & Combust.* **85**, 549-566.

We examine the support for the Batchelor spectrum from well-resolved simulations of high-Schmidt-number mixing in isotropic turbulence, and resolve a conundrum with respect to the numerical value of the prefactor, also known as the Batchelor constant. Our conclusion is that the most probable value of the most compressive principal strain rate is more relevant than its mean, at least asymptotically.

KADOCH, B., IYER, K.P., DONZIS, D.A., SCHNEIDER, K., FARGE, M. & YEUNG, P.K. (2011) On the role of vortical structures for turbulent mixing using direct numerical simulation and wavelet-based coherent vortex extraction. *J. Turbulence* **12**, doi:10.1080/14685248.2011.562511 (17 pages).

The influence of vortical structures on the transport and mixing of passive scalars is investigated. Initial conditions are taken from a direct numerical simulation database of forced homogeneous isotropic turbulence, with passive scalar fluctuations, driven by a uniform mean gradient, are performed for Taylor microscale Reynolds numbers ( $R_\lambda$ ) of 140 and 240, and Schmidt numbers  $1/8$  and  $1$ . For each  $R$ , after reaching a fully developed turbulent regime, which is statistically steady, the Coherent Vorticity Extraction is applied to the flow. It is shown that the coherent part is able to preserve the vortical structures with only less than 4% of wavelet coefficients while retaining 99.9% of energy. In contrast, the incoherent part is structureless and contains negligible energy. By taking the total, coherent and incoherent velocity fields in turn as initial conditions, new simulations were performed without forcing while the uniform mean scalar gradient

is maintained. It is found that the results from simulations with total and coherent velocity fields as initial conditions are very similar. In contrast, the time integration of the incoherent flow exhibits its primarily dissipative nature. The evolutions of passive scalars at Schmidt numbers  $1/8$  and  $1$  advected by the total, coherent or incoherent velocity suggest that the vortical structures retained in the coherent part play a dominant role in turbulent transport and mixing. Indeed, the total and coherent flows give almost the same time evolution of the scalar variance, scalar flux and mean scalar dissipation, while the incoherent flow only gives rise to weak scalar diffusion.

HACKL, J.F., YEUNG, P.K. & SAWFORD, B.L. (2011) Multi-particle and tetrad statistics in numerical simulations of turbulent relative dispersion. *Phys. Fluids* **23**, 065103 (20 pages).

The evolution in size and shape of three and four-particle clusters (triangles and tetrads, respectively) in isotropic turbulence is studied using direct numerical simulations at grid resolution up to  $4096^3$  and Taylor-scale Reynolds numbers from 140 to 1000. A key issue is the attainment of inertial range behavior at high Reynolds number, while the small- and large-time limits of ballistic and diffusive regimes respectively are also considered in some detail. Tetrad size expressed by the volume ( $V$ ) and (more appropriately) the gyration radius ( $R$ ) is shown to display inertial range scaling consistent with a Richardson constant close to 0.56 for two-particle relative dispersion. For tetrads of initial size in suitable range moments of shape parameters, including the ratio  $V^{2/3}/R^2$  and normalized eigenvalues of a moment-of-inertia-like dispersion tensor, show a regime of near-constancy which is identified with inertial-range scaling. Sheet-like structures are dominant in this period, while pancakes and needles are more prevalent at later times. For triangles taken from different faces of each tetrad effects of the initial shape (isosceles right-angled or equilateral) are retained only for about one Batchelor time scale. In the inertial range there is a prevalence of nearly isosceles triangles of two long sides and one short side, representing one particle moving away from the other two which are still close together. In general, measures of shape display asymptotic scaling ranges more readily than measures of size. With some caveats, the simulation results are also compared with the limited literature available for multiparticle cluster dispersion in turbulent flow.

DONZIS, D.A., SREENIVASAN, K.R. & YEUNG, P.K. (2011) Some results on the Reynolds number scaling of pressure statistics in isotropic turbulence. *Physica D* (in press, doi:10.1016/j.physd.2011.04.015).

Using data from direct numerical simulations in the Reynolds number range  $8 \leq R_\lambda \leq 1000$ , where  $R_\lambda$  is the Taylor microscale Reynolds number, we assess the Reynolds number scaling of the microscale and the integral length scale of pressure fluctuations in homogeneous and isotropic turbulence. The rootmean-square (rms) pressure (in kinematic units) is about  $0.91 \rho u'^2$ , where  $u$  is the rms velocity in any one direction. The ratio of the pressure microscale to the (longitudinal) velocity Taylor microscale is a constant of about 0.74 for very low Reynolds numbers but increases approximately as  $0.17 R_\lambda^{1/3}$  at high Reynolds numbers. We discuss these results in the context of the existing theory and provide plausible explanations, based on intermittency, for their observed trends.

SAWFORD, B.L. & YEUNG, P.K. (2011) Kolmogorov similarity scaling for one-particle Lagrangian statistics. *Phys. Fluids* **23**, 091704 (4 pages).

We use direct numerical simulation data up to a Taylor scale Reynolds number  $R_\lambda = 1000$  to investigate Kolmogorov similarity scaling in the inertial sub-range for one-particle Lagrangian statistics. Although similarity scaling is not achieved at these Reynolds numbers for the Lagrangian velocity structure function, we show clearly that it is achieved for the Lagrangian acceleration spectrum and the scaling range increases with Reynolds number. Stochastic and heuristic model calculations suggest that the different behaviour observed for the structure function and spectrum is simply a consequence of different rates of convergence to scaling behaviour with increasing Reynolds number. Our estimate  $C_0 \approx 7 \pm 0.2$  for the Lagrangian structure function constant is close to earlier estimates based on extrapolation of the peak value of the compensated structure function.

BLUM, D.B., BEWLEY, G.P., BODENSCHATZ, E., GILBERT, M., GYLFASSON, A., MYDLARSKI, L., VOTH, G.A., XU, H. & YEUNG, P.K. (2011) Signatures of non-universal large scales in conditional structure functions from various turbulent flows *New J. Phys.* (in press)

We present a systematic comparison of conditional structure functions in nine turbulent flows. The flows studied include forced isotropic turbulence simulated on a periodic domain, passive grid wind tunnel turbulence in air and in pressurized  $SF_6$ , active grid wind tunnel turbulence (in both synchronous and random driving modes), the flow between counter-rotating disks, oscillating grid turbulence, and the flow in the Lagrangian exploration module (in both constant and random driving modes). We compare longitudinal Eulerian second-order structure functions conditioned on the instantaneous large-scale velocity in each flow to assess the ways in which the large scales affect the small scales in a variety of turbulent flows. Structure functions are shown to have larger values when the large-scale velocity significantly deviates from the mean in most flows suggesting that dependence on the large scales is typical in many turbulent flows. The effects of the large-scale velocity on the structure functions can be quite dramatic, with the structure function varying by up to a factor of 2 when the large-scale velocity deviates from the mean by  $\pm 2$  standard deviations. In several flows, the effects of the large-scale velocity are similar at all the length scales we measured, indicating that the large-scale effects are scale independent. In a few flows, the effects of the large-scale velocity are larger on the smallest length scales.